Large Scale Modelling of Photo-Excitation Processes in Materials with Application in Organic Photovoltaics

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Propositions

belonging to the PhD thesis entitled

Large Scale Modelling of Photo-Excitation Processes in Materials with Application in Organic Photovoltaics

of

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1) The HOMO-LUMO gap in the Kohn-Sham model is, with respect to Hartree-Fock, neither wrong nor underestimated *(E. J. Baerends, O. V. Gritsenko, R. van Meer, Phys. Chem. Chem. Phys. 15:164408, 2013)*.

2) The notion of size-consistency is a purely chemical concept *(M. Nooijen*, K. R. Shamasundar, D. Mukherjee, Mol. Phys. 103:2277, 2005)*.

3) Understanding that our "understanding" might be wrong should be the cornerstone of scientific research.

4) The near-degeneracy problem is not solved by standard configurational mixing but by multiconfigurational self-consistent field theory *(B. O. Roos, Int. J. Quant. Chem. 18:175, 1980)*.

5) The development of technologies for organic photovoltaics remains largely empirical due to the difficulties in simulating device current density-voltage characteristics of optoelectronic materials *(J. Nelson, Mat. Today, 14:462, 2011)*.

6) Theory, experimentation, modelling and data science are the four fundamental branches of modern research.

7) A scientist's desire to know and learn resembles the enthalpy and entropy of a thermodynamic system.

8) A promotor is to a student what a photon is to an electron.

9) Prime numbers are building blocks of mathematics like atoms are building blocks of matter.